

*C.1 Inviscid Fluxes*

The spatial derivatives of the convective and pressure terms are written conservatively as a flux balance across a cell as, for example,

$$(\delta_\xi \hat{\mathbf{F}})_i = \hat{\mathbf{F}}_{i+\frac{1}{2}} - \hat{\mathbf{F}}_{i-\frac{1}{2}} \quad (\text{C-1})$$

where the i index denotes a cell-center location and $i \pm 1/2$ corresponds to a cell-interface location. The interface flux is determined from a state-variable interpolation and a locally one-dimensional flux model. For flux-vector splitting (FVS), Equation (C-1) is split into forward and backward-moving pieces as:

$$(\delta_\xi \hat{\mathbf{F}})_i = (\delta_\xi^- \hat{\mathbf{F}}^+ + \delta_\xi^+ \hat{\mathbf{F}}^-)_i = [\hat{\mathbf{F}}^+(\mathbf{q}_L) + \hat{\mathbf{F}}^-(\mathbf{q}_R)]_{i+\frac{1}{2}} - [\hat{\mathbf{F}}^+(\mathbf{q}_L) + \hat{\mathbf{F}}^-(\mathbf{q}_R)]_{i-\frac{1}{2}} \quad (\text{C-2})$$

For flux-difference splitting (FDS), the interface flux is written as an exact solution to an approximate Riemann problem as:

$$\begin{aligned} (\delta_\xi \hat{\mathbf{F}})_i = & \frac{1}{2} [\hat{\mathbf{F}}(\mathbf{q}_L) + \hat{\mathbf{F}}(\mathbf{q}_R) - |\tilde{\mathbf{A}}_{\text{inv}}|(\mathbf{q}_R - \mathbf{q}_L)]_{i+\frac{1}{2}} \\ & - \frac{1}{2} [\hat{\mathbf{F}}(\mathbf{q}_L) + \hat{\mathbf{F}}(\mathbf{q}_R) - |\tilde{\mathbf{A}}_{\text{inv}}|(\mathbf{q}_R - \mathbf{q}_L)]_{i-\frac{1}{2}} \end{aligned} \quad (\text{C-3})$$

Further details on the FVS and FDS methods are given below. In both cases, interpolated values \mathbf{q}_L and \mathbf{q}_R at each interface are required. The state variable interpolations determine the resulting accuracy of the scheme. They are constructed from interpolation of the primitive variables. For first-order fully-upwind differencing:

$$\begin{aligned} (\mathbf{q}_L)_{i+\frac{1}{2}} &= \mathbf{q}_i \\ (\mathbf{q}_R)_{i+\frac{1}{2}} &= \mathbf{q}_{i+1} \end{aligned} \quad (\text{C-4})$$

Higher order accuracy is given by the family of interpolations:

$$\begin{aligned}
(\mathbf{q}_L)_{i+\frac{1}{2}} &= \mathbf{q}_i + \frac{1}{4}[(1-\kappa)\Delta_- + (1+\kappa)\Delta_+]_i \\
(\mathbf{q}_R)_{i+\frac{1}{2}} &= \mathbf{q}_{i+1} - \frac{1}{4}[(1-\kappa)\Delta_+ + (1+\kappa)\Delta_-]_{i+1}
\end{aligned}
\tag{C-5}$$

where

$$\begin{aligned}
\Delta_+ &\equiv \mathbf{q}_{i+1} - \mathbf{q}_i \\
\Delta_- &\equiv \mathbf{q}_i - \mathbf{q}_{i-1}
\end{aligned}
\tag{C-6}$$

The parameter $\kappa \in [-1, 1]$ forms a family of difference schemes. $\kappa = -1$ corresponds to second-order fully-upwind differencing, $\kappa = 1/3$ to third-order upwind-biased differencing, and $\kappa = 1$ to central differencing. Note, however, that setting $\kappa = 1$ in CFL3D will result in odd-even point decoupling, since there is no artificial dissipation in the code. Also note that “third order” for $\kappa = 1/3$ is only obtained for one-dimensional flows. For two and three dimensions, the formal order of accuracy is second order.

In practice, the gradients of density and pressure are biased by an average value in order to improve the robustness of the calculation at higher Mach numbers and in the early transient stages of a solution.

$$\begin{aligned}
\Delta_+^b &= \frac{\Delta_+}{\mathbf{q}_i + \frac{1}{2}\Delta_+} \\
\Delta_-^b &= \frac{\Delta_-}{\mathbf{q}_i - \frac{1}{2}\Delta_-}
\end{aligned}
\tag{C-7}$$

And,

$$\begin{aligned}
(\mathbf{q}_L)_{i+\frac{1}{2}} &= \mathbf{q}_i + \frac{\mathbf{q}_i}{4}[(1-\kappa)\Delta_-^b + (1+\kappa)\Delta_+^b]_i \\
(\mathbf{q}_R)_{i+\frac{1}{2}} &= \mathbf{q}_{i+1} - \frac{\mathbf{q}_{i+1}}{4}[(1-\kappa)\Delta_+^b + (1+\kappa)\Delta_-^b]_{i+1}
\end{aligned}
\tag{C-8}$$

Note that Equation (C-8) is not performed for the gradients of velocity; this is essentially an extrapolation of the log of the density and pressure (first-order expansion).

C.1.1 Flux Limiting

For solutions with discontinuities (such as shock waves), schemes of order higher than one generally require a flux limiter to avoid numerical oscillations in the solution. CFL3D has several limiter options.

The smooth limiter (**iflim** = 1) is implemented via

$$\begin{aligned} (\mathbf{q}_L)_{i+\frac{1}{2}} &= \mathbf{q}_i + \left\{ \frac{s}{4} [(1 - \kappa s)\Delta_- + (1 + \kappa s)\Delta_+] \right\}_i \\ (\mathbf{q}_R)_{i+\frac{1}{2}} &= \mathbf{q}_{i+1} - \left\{ \frac{s}{4} [(1 - \kappa s)\Delta_+ + (1 + \kappa s)\Delta_-] \right\}_{i+1} \end{aligned} \quad (\text{C-9})$$

where

$$s = \frac{2\Delta_+\Delta_- + \varepsilon}{(\Delta_+)^2 + (\Delta_-)^2 + \varepsilon} \quad (\text{C-10})$$

and ε is a small number ($\varepsilon = 1 \times 10^{-6}$) preventing division by zero in regions of null gradient.

The min-mod limiter (**iflim** = 2) is implemented via

$$\begin{aligned} (\mathbf{q}_L)_{i+\frac{1}{2}} &= \mathbf{q}_i + \frac{1}{4} [(1 - \kappa)\bar{\Delta}_- + (1 + \kappa)\bar{\Delta}_+]_i \\ (\mathbf{q}_R)_{i+\frac{1}{2}} &= \mathbf{q}_{i+1} - \frac{1}{4} [(1 - \kappa)\bar{\Delta}_+ + (1 + \kappa)\bar{\Delta}_-]_{i+1} \end{aligned} \quad (\text{C-11})$$

where

$$\begin{aligned} \bar{\Delta}_- &= \text{minmod}(\Delta_-, b\Delta_+) \\ \bar{\Delta}_+ &= \text{minmod}(\Delta_+, b\Delta_-) \end{aligned} \quad (\text{C-12})$$

$$\text{minmod}(x, y) = \max\{0, \min[x \text{ sign}(y), b \text{ sign}(x)]\} \text{ sign}(x) \quad (\text{C-13})$$

The parameter b is a compression parameter, $b = (3 - \kappa)/(1 - \kappa)$.

The smooth limiter tuned to $\kappa = 1/3$ (**iflim** = 3) is implemented as follows.

$$\begin{aligned}
(\mathbf{q}_L)_{i+\frac{1}{2}} &= \mathbf{q}_i + \frac{1}{2}(\delta_L \mathbf{q})_i \\
(\mathbf{q}_R)_{i+\frac{1}{2}} &= \mathbf{q}_{i+1} - \frac{1}{2}(\delta_R \mathbf{q})_{i+1}
\end{aligned} \tag{C-14}$$

where

$$\begin{aligned}
(\delta_L \mathbf{q})_i &= I(\mathbf{q}_{i+1} - \mathbf{q}_i, \mathbf{q}_i - \mathbf{q}_{i-1}) \\
(\delta_R \mathbf{q})_i &= I(\mathbf{q}_i - \mathbf{q}_{i-1}, \mathbf{q}_{i+1} - \mathbf{q}_i)
\end{aligned} \tag{C-15}$$

$$I(x, y) = \frac{x(y^2 + 2\epsilon^2) + y(2x^2 + \epsilon^2)}{2x^2 - xy + 2y^2 + 3\epsilon^2} \tag{C-16}$$

and I is designed to recover the state variable to third-order accuracy in the one-dimensional case in smooth regions of the flow and interpolate without oscillations near discontinuities. The parameter ϵ^2 is a small constant of order Δx^3 which is used to improve the accuracy near smooth extremum and reduce the nonlinearity of the interpolation in regions of small gradient.

C.1.2 Flux-Vector Splitting

The flux-vector splitting (FVS) method of van Leer³⁹ is implemented as follows. The generalized inviscid fluxes $\hat{\mathbf{F}}$, $\hat{\mathbf{G}}$, and $\hat{\mathbf{H}}$, representing the pressure and convection terms, are upwind differenced by splitting into forward and backward contributions and differencing accordingly. For example, the flux difference in the ξ direction is

$$\delta_\xi \hat{\mathbf{F}} = \delta_\xi^- \hat{\mathbf{F}}^+ + \delta_\xi^+ \hat{\mathbf{F}}^- \tag{C-17}$$

where δ_ξ^- and δ_ξ^+ denote general backward and forward divided difference operators, respectively. For flux-vector splitting, $\hat{\mathbf{F}}$ is split according to the contravariant Mach number in the ξ direction, defined as

$$M_\xi = \frac{\bar{U}}{a} \tag{C-18}$$

where

$$\bar{U} = \frac{U}{|\nabla \xi|} \tag{C-19}$$

and

$$U = \xi_x u + \xi_y v + \xi_z w + \xi_t \quad (\text{C-20})$$

For locally supersonic flow, where $|M_\xi| \geq 1$,

$$\begin{aligned} \hat{\mathbf{F}}^+ &= \hat{\mathbf{F}} & \hat{\mathbf{F}}^- &= 0 & M_\xi &\geq +1 \\ \hat{\mathbf{F}}^- &= \hat{\mathbf{F}} & \hat{\mathbf{F}}^+ &= 0 & M_\xi &\leq -1 \end{aligned} \quad (\text{C-21})$$

and for locally subsonic flow, where $|M_\xi| < 1$,

$$\hat{\mathbf{F}} = \frac{|\nabla \xi|}{J} \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \end{bmatrix} = \frac{|\nabla \xi|}{J} \begin{bmatrix} f_{\text{mass}} \\ f_{\text{mass}}[\hat{\xi}_x(-\bar{U} \pm 2a)/\gamma + u] \\ f_{\text{mass}}[\hat{\xi}_y(-\bar{U} \pm 2a)/\gamma + v] \\ f_{\text{mass}}[\hat{\xi}_z(-\bar{U} \pm 2a)/\gamma + w] \\ f_{\text{energy}} \end{bmatrix} \quad (\text{C-22})$$

where the direction cosines of the cell interfaces are

$$\hat{\xi}_x = \frac{\xi_x}{|\nabla \xi|} \quad \hat{\xi}_y = \frac{\xi_y}{|\nabla \xi|} \quad \hat{\xi}_z = \frac{\xi_z}{|\nabla \xi|} \quad (\text{C-23})$$

and

$$f_{\text{mass}} = \pm \frac{\rho a}{4} (M_\xi \pm 1)^2 \quad (\text{C-24})$$

$$f_{\text{energy}} = f_{\text{mass}} \left[\frac{(1-\gamma)\bar{U}^2 \pm 2(\gamma-1)\bar{U}a + 2a^2}{(\gamma^2-1)} + \frac{(u^2 + v^2 + w^2)}{2} - \frac{\hat{\xi}_t}{\gamma}(-\bar{U} \pm 2a) \right] \quad (\text{C-25})$$

and

$$\hat{\xi}_t = \frac{\xi_t}{|\nabla \xi|} \quad (\text{C-26})$$

For an implicit scheme, the Jacobians of the right-hand-side flux terms must be determined (see Appendix B). They appear as terms in the left-hand-side matrix multiplying $\Delta \mathbf{q}$, and the resulting system of equations is solved with a full 5 by 5 block-tridiagonal

inversion procedure. For flux-vector splitting, the split flux Jacobians (with respect to the primitive variables) for the ξ direction, i.e. $\frac{\partial \hat{\mathbf{F}}}{\partial \mathbf{q}}$, are

$$\begin{aligned}
 \frac{\partial F_1}{\partial \rho} &= \frac{1}{4}(\bar{U} \pm a) \left[-1 \pm \frac{3}{2a}(\bar{U} \pm a) \right] \\
 \frac{\partial F_1}{\partial u} &= \pm \frac{\rho}{2a}(\bar{U} \pm a) \hat{\xi}_x \\
 \frac{\partial F_1}{\partial v} &= \pm \frac{\rho}{2a}(\bar{U} \pm a) \hat{\xi}_y \\
 \frac{\partial F_1}{\partial w} &= \pm \frac{\rho}{2a}(\bar{U} \pm a) \hat{\xi}_z \\
 \frac{\partial F_1}{\partial p} &= \frac{-\gamma}{4a^2}(\bar{U} \pm a) \left[-1 \pm \frac{1}{2a}(\bar{U} \pm a) \right]
 \end{aligned} \tag{C-27}$$

$$\begin{aligned}
 \frac{\partial F_2}{\partial \rho} &= \pm \frac{1}{4}(\bar{U} \pm a) \left[\frac{3\bar{U}}{2a\gamma}(-\bar{U} \pm a) \hat{\xi}_x + u \left(\frac{3}{2a}(\bar{U} \pm a) \mp 1 \right) \right] \\
 \frac{\partial F_2}{\partial u} &= \pm \frac{\rho}{4a}(\bar{U} \pm a) \left[\hat{\xi}_x \left(\frac{3\hat{\xi}_x}{\gamma}(-\bar{U} \pm a) + 2u \right) + (\bar{U} \pm a) \right] \\
 \frac{\partial F_2}{\partial v} &= \pm \frac{\rho}{4a}(\bar{U} \pm a) \hat{\xi}_y \left[\frac{3\hat{\xi}_x}{\gamma}(-\bar{U} \pm a) + 2u \right] \\
 \frac{\partial F_2}{\partial w} &= \pm \frac{\rho}{4a}(\bar{U} \pm a) \hat{\xi}_z \left[\frac{3\hat{\xi}_x}{\gamma}(-\bar{U} \pm a) + 2u \right] \\
 \frac{\partial F_2}{\partial p} &= \pm \frac{1}{4a^2}(\bar{U} \pm a) \left\{ \hat{\xi}_x \left[2a - \frac{\bar{U}}{2a}(-\bar{U} \pm a) \pm \gamma u \left(1 \mp \frac{1}{2a}(\bar{U} \pm a) \right) \right] \right\}
 \end{aligned} \tag{C-28}$$

$$\begin{aligned}
\frac{\partial F_3}{\partial \rho} &= \pm \frac{1}{4}(\bar{U} \pm a) \left[\frac{3\bar{U}}{2a\gamma}(-\bar{U} \pm a)\hat{\xi}_y + v \left(\frac{3}{2a}(\bar{U} \pm a) \mp 1 \right) \right] \\
\frac{\partial F_3}{\partial u} &= \pm \frac{\rho}{4a}(\bar{U} \pm a)\hat{\xi}_x \left[\frac{3\hat{\xi}_y}{\gamma}(-\bar{U} \pm a) + 2v \right] \\
\frac{\partial F_3}{\partial v} &= \pm \frac{\rho}{4a}(\bar{U} \pm a) \left[\hat{\xi}_y \left(\frac{3\hat{\xi}_y}{\gamma}(-\bar{U} \pm a) + 2v \right) + (\bar{U} \pm a) \right] \\
\frac{\partial F_3}{\partial w} &= \pm \frac{\rho}{4a}(\bar{U} \pm a)\hat{\xi}_z \left[\frac{3\hat{\xi}_y}{\gamma}(-\bar{U} \pm a) + 2v \right] \\
\frac{\partial F_3}{\partial p} &= \pm \frac{1}{4a^2}(\bar{U} \pm a) \left\{ \hat{\xi}_y \left[2a - \frac{\bar{U}}{2a}(-\bar{U} \pm a) \pm \gamma v \left(1 \mp \frac{1}{2a}(\bar{U} \pm a) \right) \right] \right\}
\end{aligned} \tag{C-29}$$

$$\begin{aligned}
\frac{\partial F_4}{\partial \rho} &= \pm \frac{1}{4}(\bar{U} \pm a) \left[\frac{3\bar{U}}{2a\gamma}(-\bar{U} \pm a)\hat{\xi}_z + w \left(\frac{3}{2a}(\bar{U} \pm a) \mp 1 \right) \right] \\
\frac{\partial F_4}{\partial u} &= \pm \frac{\rho}{4a}(\bar{U} \pm a)\hat{\xi}_x \left[\frac{3\hat{\xi}_z}{\gamma}(-\bar{U} \pm a) + 2w \right] \\
\frac{\partial F_4}{\partial v} &= \pm \frac{\rho}{4a}(\bar{U} \pm a)\hat{\xi}_y \left[\frac{3\hat{\xi}_z}{\gamma}(-\bar{U} \pm a) + 2w \right] \\
\frac{\partial F_4}{\partial w} &= \pm \frac{\rho}{4a}(\bar{U} \pm a) \left[\hat{\xi}_z \left(\frac{3\hat{\xi}_z}{\gamma}(-\bar{U} \pm a) + 2w \right) + (\bar{U} \pm a) \right] \\
\frac{\partial F_4}{\partial p} &= \pm \frac{1}{4a^2}(\bar{U} \pm a) \left\{ \hat{\xi}_z \left[2a - \frac{\bar{U}}{2a}(-\bar{U} \pm a) \pm \gamma w \left(1 \mp \frac{1}{2a}(\bar{U} \pm a) \right) \right] \right\}
\end{aligned} \tag{C-30}$$

$$\begin{aligned}
\frac{\partial F_5}{\partial \rho} &= \pm \frac{1}{4}(\bar{U} \pm a) \left\{ (-\bar{U} \pm a) \left[\frac{3\bar{U}}{2a} \left(\frac{\bar{U}}{\gamma+1} - \frac{\hat{\xi}_t}{\gamma} \right) - \frac{a}{\gamma^2-1} \right] + \frac{u^2 + v^2 + w^2}{2} \left[\frac{3}{2a}(\bar{U} \pm a) \mp 1 \right] \right\} \\
\frac{\partial F_5}{\partial u} &= \pm \frac{\rho}{4a}(\bar{U} \pm a) \left\{ \hat{\xi}_x \left[\frac{2a^2}{\gamma-1} + \left(\frac{4\bar{U}}{\gamma+1} - \frac{3\hat{\xi}_t}{\gamma} \right) (-\bar{U} \pm a) + u^2 + v^2 + w^2 \right] + u(\bar{U} \pm a) \right\} \\
\frac{\partial F_5}{\partial v} &= \pm \frac{\rho}{4a}(\bar{U} \pm a) \left\{ \hat{\xi}_y \left[\frac{2a^2}{\gamma-1} + \left(\frac{4\bar{U}}{\gamma+1} - \frac{3\hat{\xi}_t}{\gamma} \right) (-\bar{U} \pm a) + u^2 + v^2 + w^2 \right] + v(\bar{U} \pm a) \right\} \\
\frac{\partial F_5}{\partial w} &= \pm \frac{\rho}{4a}(\bar{U} \pm a) \left\{ \hat{\xi}_z \left[\frac{2a^2}{\gamma-1} + \left(\frac{4\bar{U}}{\gamma+1} - \frac{3\hat{\xi}_t}{\gamma} \right) (-\bar{U} \pm a) + u^2 + v^2 + w^2 \right] + w(\bar{U} \pm a) \right\}
\end{aligned} \tag{C-31}$$

$$\frac{\partial F_5}{\partial p} = \pm \frac{\gamma}{4a} (\bar{U} \pm a) \left\{ \left[\left(\frac{\bar{U}}{\gamma+1} - \frac{\hat{\xi}_t}{\gamma} \right) \left(2a - \frac{\bar{U}}{2a} (-\bar{U} \pm a) \right) + \frac{a}{\gamma^2 - 1} (\bar{U} \pm 3a) + \frac{u^2 + v^2 + w^2}{2} \left(-\frac{1}{2a} (\bar{U} \pm a) \pm 1 \right) \right] \right\}$$

C.1.3 Flux-Difference Splitting

In the flux-difference splitting (FDS) method of Roe³¹, the interface flux in the ξ direction is written

$$\hat{\mathbf{F}}_{i+\frac{1}{2}} = \frac{1}{2} [\hat{\mathbf{F}}(\mathbf{q}_L) + \hat{\mathbf{F}}(\mathbf{q}_R) - |\tilde{\mathbf{A}}_{\text{inv}}|(\mathbf{q}_R - \mathbf{q}_L)]_{i+\frac{1}{2}} \quad (\text{C-32})$$

where $\tilde{\mathbf{A}}_{\text{inv}}$ is \mathbf{A}_{inv} evaluated with Roe-averaged variables defined below. (\mathbf{A}_{inv} is the inviscid part of the \mathbf{A} matrix defined in Appendix B.) Hence,

$$|\tilde{\mathbf{A}}_{\text{inv}}| = |\mathbf{A}_{\text{inv}}(\tilde{\mathbf{q}})| \quad (\text{C-33})$$

and

$$\begin{aligned} \tilde{\mathbf{q}} &= \tilde{\mathbf{q}}(\mathbf{q}_L, \mathbf{q}_R) \\ \mathbf{A}_{\text{inv}} &= \frac{\partial \hat{\mathbf{F}}}{\partial \mathbf{Q}} = \mathbf{T} \Lambda \mathbf{T}^{-1} = \mathbf{T}(\Lambda^+ + \Lambda^-) \mathbf{T}^{-1} \\ \Lambda &= \frac{\Lambda \pm |\Lambda|}{2} \\ |\mathbf{A}_{\text{inv}}| &= \mathbf{T} |\Lambda| \mathbf{T}^{-1} \end{aligned} \quad (\text{C-34})$$

The diagonal matrix Λ is the matrix of eigenvalues of \mathbf{A}_{inv} , \mathbf{T} is the matrix of right eigenvectors as columns, and \mathbf{T}^{-1} is the matrix of left eigenvectors as rows. They are all evaluated at Roe-averaged values such that

$$\hat{\mathbf{F}}(\mathbf{Q}_R) - \hat{\mathbf{F}}(\mathbf{Q}_L) = \tilde{\mathbf{A}}_{\text{inv}}(\mathbf{Q}_R - \mathbf{Q}_L) \quad (\text{C-35})$$

is satisfied exactly. The term $|\tilde{\mathbf{A}}_{\text{inv}}|(\mathbf{Q}_R - \mathbf{Q}_L)$ can be written

$$|\tilde{\mathbf{A}}_{\text{inv}}|(\mathbf{Q}_R - \mathbf{Q}_L) \equiv |\tilde{\mathbf{A}}_{\text{inv}}|\Delta\mathbf{Q} = \begin{bmatrix} \alpha_4 \\ \tilde{u}\alpha_4 + \hat{\xi}_x\alpha_5 + \alpha_6 \\ \tilde{v}\alpha_4 + \hat{\xi}_y\alpha_5 + \alpha_7 \\ \tilde{w}\alpha_4 + \hat{\xi}_z\alpha_5 + \alpha_8 \\ \tilde{H}\alpha_4 + (\tilde{U} - \hat{\xi}_t)\alpha_5 + \tilde{u}\alpha_6 + \tilde{v}\alpha_7 + \tilde{w}\alpha_8 - \frac{\tilde{a}^2\alpha_1}{\gamma-1} \end{bmatrix} \quad (\text{C-36})$$

where

$$\begin{aligned} \alpha_1 &= \left| \frac{\nabla \xi}{J} \right| |\tilde{U}| \left(\Delta\rho - \frac{\Delta p}{\tilde{a}^2} \right) \\ \alpha_2 &= \frac{1}{2\tilde{a}^2} \left| \frac{\nabla \xi}{J} \right| |\tilde{U} + \tilde{a}| (\Delta p + \tilde{\rho}\tilde{a}\Delta\bar{U}) \\ \alpha_3 &= \frac{1}{2\tilde{a}^2} \left| \frac{\nabla \xi}{J} \right| |\tilde{U} - \tilde{a}| (\Delta p - \tilde{\rho}\tilde{a}\Delta\bar{U}) \\ \alpha_4 &= \alpha_1 + \alpha_2 + \alpha_3 \\ \alpha_5 &= \tilde{a}(\alpha_2 - \alpha_3) \\ \alpha_6 &= \left| \frac{\nabla \xi}{J} \right| |\tilde{U}| (\tilde{\rho}\Delta u - \hat{\xi}_x\tilde{\rho}\Delta\bar{U}) \\ \alpha_7 &= \left| \frac{\nabla \xi}{J} \right| |\tilde{U}| (\tilde{\rho}\Delta v - \hat{\xi}_y\tilde{\rho}\Delta\bar{U}) \\ \alpha_8 &= \left| \frac{\nabla \xi}{J} \right| |\tilde{U}| (\tilde{\rho}\Delta w - \hat{\xi}_z\tilde{\rho}\Delta\bar{U}) \end{aligned} \quad (\text{C-37})$$

Here, the notation \sim denotes the following Roe-averaged evaluations:

$$\begin{aligned}
 \tilde{\rho} &= \sqrt{\rho_L \rho_R} \\
 \tilde{u} &= \frac{u_L + u_R \sqrt{\rho_R / \rho_L}}{1 + \sqrt{\rho_R / \rho_L}} \\
 \tilde{v} &= \frac{v_L + v_R \sqrt{\rho_R / \rho_L}}{1 + \sqrt{\rho_R / \rho_L}} \\
 \tilde{w} &= \frac{w_L + w_R \sqrt{\rho_R / \rho_L}}{1 + \sqrt{\rho_R / \rho_L}} \\
 \tilde{H} &= \frac{H_L + H_R \sqrt{\rho_R / \rho_L}}{1 + \sqrt{\rho_R / \rho_L}} \\
 \tilde{a}^2 &= (\gamma - 1) \tilde{H} - \frac{\tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2}{2}
 \end{aligned} \tag{C-38}$$

The terms $\hat{\xi}_x, \hat{\xi}_y, \hat{\xi}_z, \hat{\xi}_t$ and \bar{U} are defined in Section C.1.2 and

$$\tilde{U} = \frac{1}{|\nabla \xi|} (\xi_x \tilde{u} + \xi_y \tilde{v} + \xi_z \tilde{w} + \xi_t) \tag{C-39}$$

For flux-difference splitting, the true Jacobians are expensive to compute. Two alternatives are employed in CFL3D. When the system of equations is solved with a full 5 by 5 block-tridiagonal inversion procedure (**idiag** = 0), the following approximations for the left-hand-side flux-difference splitting Jacobians are employed:

$$\begin{aligned}
 (\mathbf{A}_{\text{inv}}^+)_{i+\frac{1}{2}} &= \frac{1}{2} \left[(\mathbf{A}_{\text{inv}})_i + |\tilde{\mathbf{A}}_{\text{inv}}|_{i+\frac{1}{2}} \right] \\
 (\mathbf{A}_{\text{inv}}^-)_{i+\frac{1}{2}} &= \frac{1}{2} \left[(\mathbf{A}_{\text{inv}})_{i+1} - |\tilde{\mathbf{A}}_{\text{inv}}|_{i+\frac{1}{2}} \right]
 \end{aligned} \tag{C-40}$$

Flux-difference splitting also has an option to employ a diagonal approximation for the left-hand side (**idiag** = 1). In this method, each of the spatial factors is approximated with a diagonal inversion as

$$\left[\frac{\mathbf{I}}{J\Delta t} + \delta_\xi \frac{\partial \mathbf{F}}{\partial \mathbf{Q}} \right] \Delta \mathbf{Q} \approx \mathbf{T} \left[\frac{\mathbf{I}}{J\Delta t} + \delta_\xi^- \Lambda^+ + \delta_\xi^+ \Lambda^- \right] \mathbf{T}^{-1} \Delta \mathbf{Q} \tag{C-41}$$

Because of the repeated eigenvalues of Λ , only three scalar tridiagonal LU decompositions are needed in each direction, resulting in a significant savings in run time.

C.2 Viscous Fluxes

The viscous terms, which represent shear stress and heat transfer effects, are discretized with second-order central differences. The second derivatives are treated as differences across cell interfaces of first-derivative terms. Hence, in the ξ direction for example, the viscous terms are discretized as

$$\delta_\xi(\hat{\mathbf{F}}_v)_i = (\hat{\mathbf{F}}_v)_{i+\frac{1}{2}} - (\hat{\mathbf{F}}_v)_{i-\frac{1}{2}} \quad (\text{C-42})$$

The term $\hat{\mathbf{F}}_v$ is given in Equation (A-8) of Appendix A. Using the thin-layer approximation, it can be written as:

$$\hat{\mathbf{F}}_v = \frac{M_\infty \mu}{Re_{\tilde{L}_R} J} \begin{bmatrix} 0 \\ \phi_1 \frac{\partial u}{\partial \xi} + \xi_x \phi_2 \\ \phi_1 \frac{\partial v}{\partial \xi} + \xi_y \phi_2 \\ \phi_1 \frac{\partial w}{\partial \xi} + \xi_z \phi_2 \\ \phi_1 \left[\delta_\xi \left(\frac{|\mathbf{V}|^2}{2} \right) + \frac{1}{Pr(\gamma-1)} \delta_\xi(a^2) \right] + (U - \xi_t) \phi_2 \end{bmatrix} \quad (\text{C-43})$$

where

$$\phi_1 = \xi_x^2 + \xi_y^2 + \xi_z^2 \quad \phi_2 = \left(\xi_x \frac{\partial u}{\partial \xi} + \xi_y \frac{\partial v}{\partial \xi} + \xi_z \frac{\partial w}{\partial \xi} \right) / 3 \quad (\text{C-44})$$

Implemented in a finite-volume approach, Equation (C-43) requires an approximation to the volume at the cell interface $(1/J)_{i+1/2}$, which is calculated by averaging the neighboring values.

When the system of equations is solved with a full 5 by 5 block-tridiagonal inversion procedure (**idiag** = 0), the viscous Jacobians (left-hand-side implicit terms) are employed only for the viscous terms in the ξ direction (corresponding with the k index of the grid). This is a hold-over from the early days of the CFL3D code, when viscous terms were employed in only one direction. Hence, keep in mind that if the **idiag** = 0 option is used when viscous terms are included in either the j or i directions, the convergence may suffer due to the lack of the appropriate left-hand-side terms. The missing left-hand-side terms have no effect on *converged* solutions, however.

However, almost all runs with CFL3D employ flux-difference splitting with the diagonal left-hand-side option (**idiag** = 1), because flux-difference splitting is generally more accurate for Navier-Stokes computations (see van Leer et al⁴¹), and **idiag** = 1 is significantly less expensive than **idiag** = 0. For the diagonal method, a spectral radius scaling for the viscous Jacobian matrices is used, similar to that developed by Coakley.¹⁴ In this reference, the true left-hand-side viscous matrix term is replaced by the matrix $\tilde{\nu}\mathbf{I}$, where \mathbf{I} is the identity matrix, $\tilde{\nu} = \tilde{\mu}_{\max}/\tilde{\rho}$, and $\tilde{\mu}_{\max}$ is the largest eigenvalue of the one-dimensional Navier-Stokes equation, $\tilde{\mu}_{\max} = \max(4\tilde{\mu}/3, \gamma\tilde{\mu}/Pr)$. In CFL3D, nondimensional μ_{\max} is taken as $2(1 + \mu_t)$, where μ_t is the nondimensional turbulent eddy viscosity.